# Benzene, beta-deuteroethynyl-

**Inchi:** InChI=1S/C8H6/c1-2-8-6-4-3-5-7-8/h1,3-7H/i1D
**InchiKey:** UEXCJVNBTNXOEH-MICDWDOJSA-N
**Formula:** C8H5D
**SMILES:** C#Cc1ccccc1
**Mol. weight [g/mol]:** 103.14

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 351.96 | kJ/mol | Joback Method |
| hf | 319.98 | kJ/mol | Joback Method |
| hfus | 13.49 | kJ/mol | Joback Method |
| hvap | 35.54 | kJ/mol | Joback Method |
| log10ws | -2.17 | | Crippen Method |
| logp | 1.668 | | Crippen Method |
| mcvol | 91.220 | ml/mol | McGowan Method |
| pc | 4403.25 | kPa | Joback Method |
| tb | 399.24 | K | Joback Method |
| tc | 625.47 | K | Joback Method |
| tf | 253.31 | K | Joback Method |
| vc | 0.338 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 149.68 | J/mol×K | 399.24 | Joback Method |
| cpg | 160.67 | J/mol×K | 436.95 | Joback Method |
| cpg | 170.89 | J/mol×K | 474.65 | Joback Method |
| cpg | 180.38 | J/mol×K | 512.36 | Joback Method |
| cpg | 189.18 | J/mol×K | 550.06 | Joback Method |
| cpg | 197.33 | J/mol×K | 587.77 | Joback Method |
| cpg | 204.88 | J/mol×K | 625.47 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=B6010137&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |